The ACTS Toolkit
Next Steps

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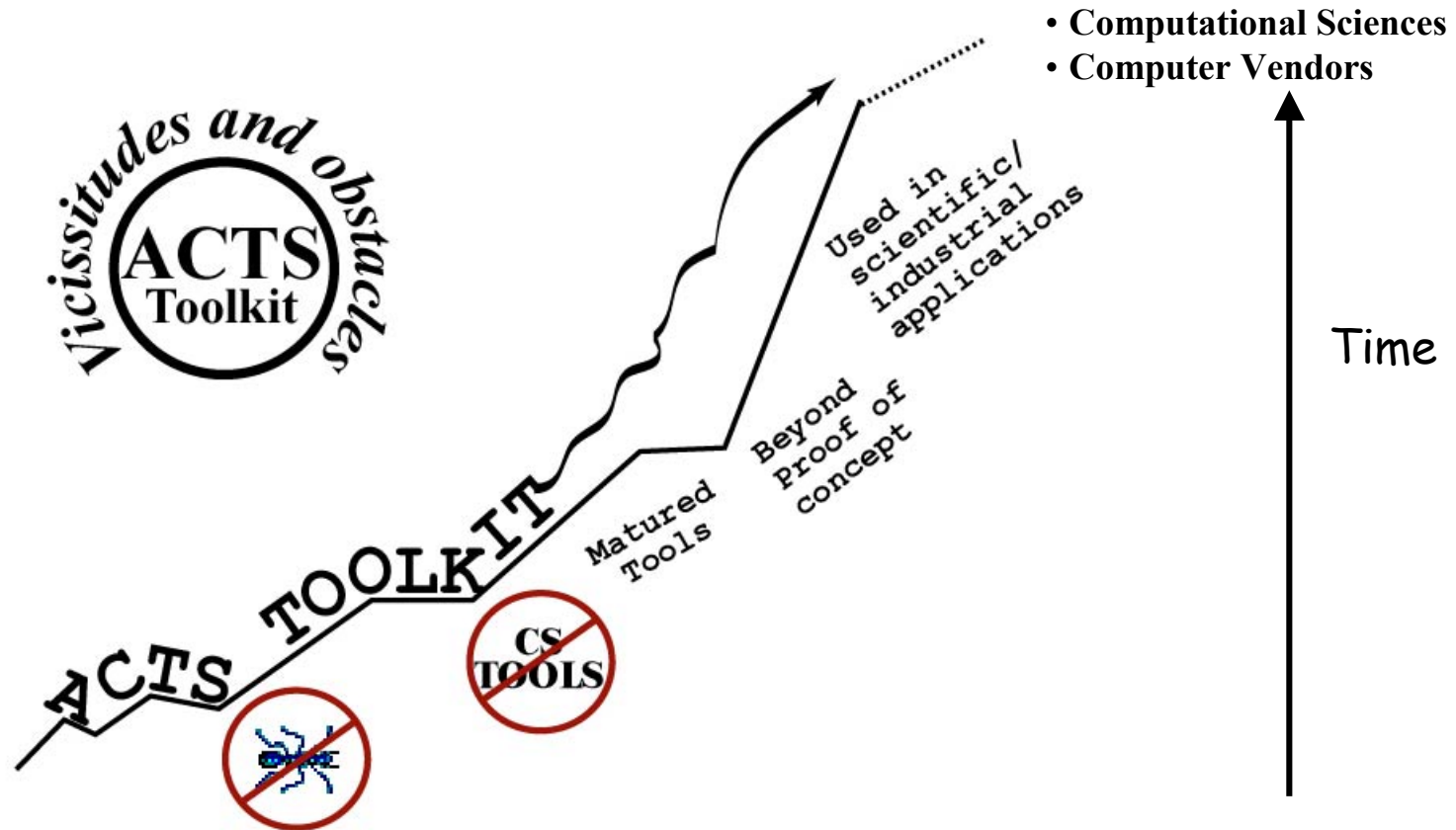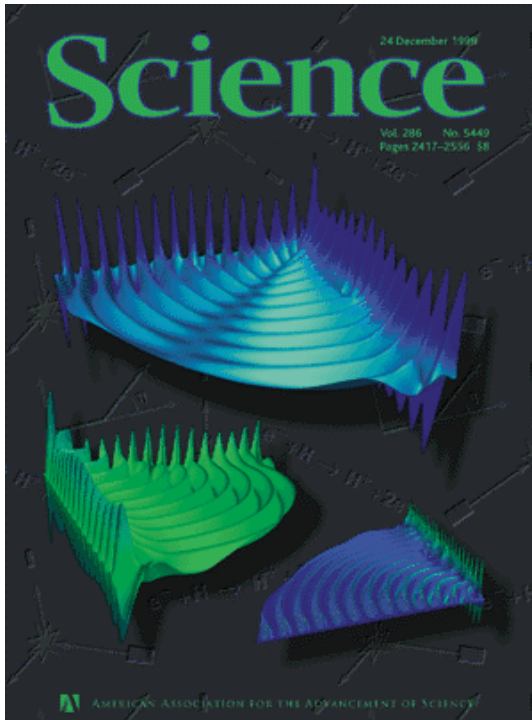
- whoswho.html

- Coming soon:

  - Pointers to related background information

  - Tutorials and hands-on exercises

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- **Computational Sciences**
- **Computer Vendors**

Time

Success Stories
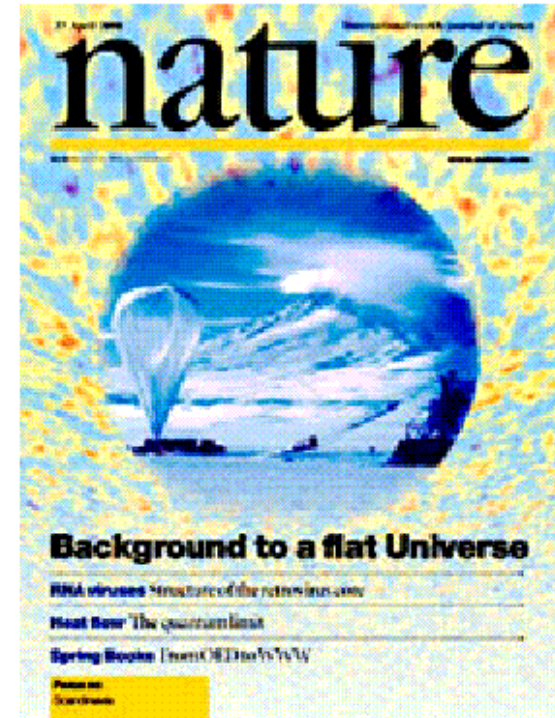
SuperLU: *Scattering in a quantum system of three charged particles (Rescigno, Baertschy, Isaacs and McCurdy, Dec. 24, 1999).*

ScaLAPACK: *Cosmic Microwave Background Analysis, BOOMERanG collaboration, MADCAP code (Apr. 27, 2000).*

What you haven't seen from ACTS yet. . .

$$Ax = b$$

(system of linear equations)

Direct Methods:

    1. $A = LU$ (L lower triangular, U upper triangular)

    2. $Ly = b$

    3. $Ux = y$

> SuperLU
> ScaLAPACK

Iterative Methods:

    $x_k = x_{k-1} + \alpha_k p_{k-1}$

    only matrix - vector multiplies are needed

    preconditoning is usually required

> Aztec/Trilinos
> Hypre
> PETSc

What needs to be computed?

$$Az = \lambda z$$

(eigenvalue problem)

ScaLAPACK

$$A = U\Sigma V^T$$

(singular value decomposition)

ScaLAPACK

$$\min\left\{\tfrac{1}{2}\left\|r(x)\right\|^2 : x_l \leq x \leq x_u\right\}$$
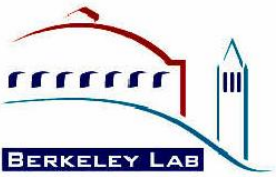
(systems of nonlinear equations)

PETSc
TAO

PDEs

PETSc

ODEs

PETSc
PVODE

- **PVODE**: solvers for large systems of ODE's

- Data structures and representations

- Computational steering

- Interactive visualization

- Distributed computation

- Data distribution and management

- Performance analysis

- Scripting Languages
  ⋮

Globus
CUMULVS
TAU
Global Arrays
PAWS
SILOON
PADRE

Structural (Frameworks)

- **POET** (Parallel Object-oriented Environment and Toolkit): allows for "mixing and matching" of components

- **POOMA** (Parallel Object-Oriented Methods and Applications): C++ abstraction layer between algorithm and platform (similar to HPF)

- **Tulip**: C++ applications with threads, global pointers and other parallel operations

- **ATLAS** (Automatically Tuned Linear Algebra Software), **PHiPAC** (Portable High Performance ANSI C): automatic generation of optimized numerical software (mainly BLAS)

- **Nexus**: multithreading, communication and resource management facilities

- **PETE** (Portable Expression Template Engine): efficient C++ operator overloading through expression templates

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Make services available from one toolkit to the other

- Solutions for a broader range of problems

- Increase visibility of a wider spectrum of computational services

- Improve code portability and further optimization

- Improve learning curves

- Benefits Computational sciences
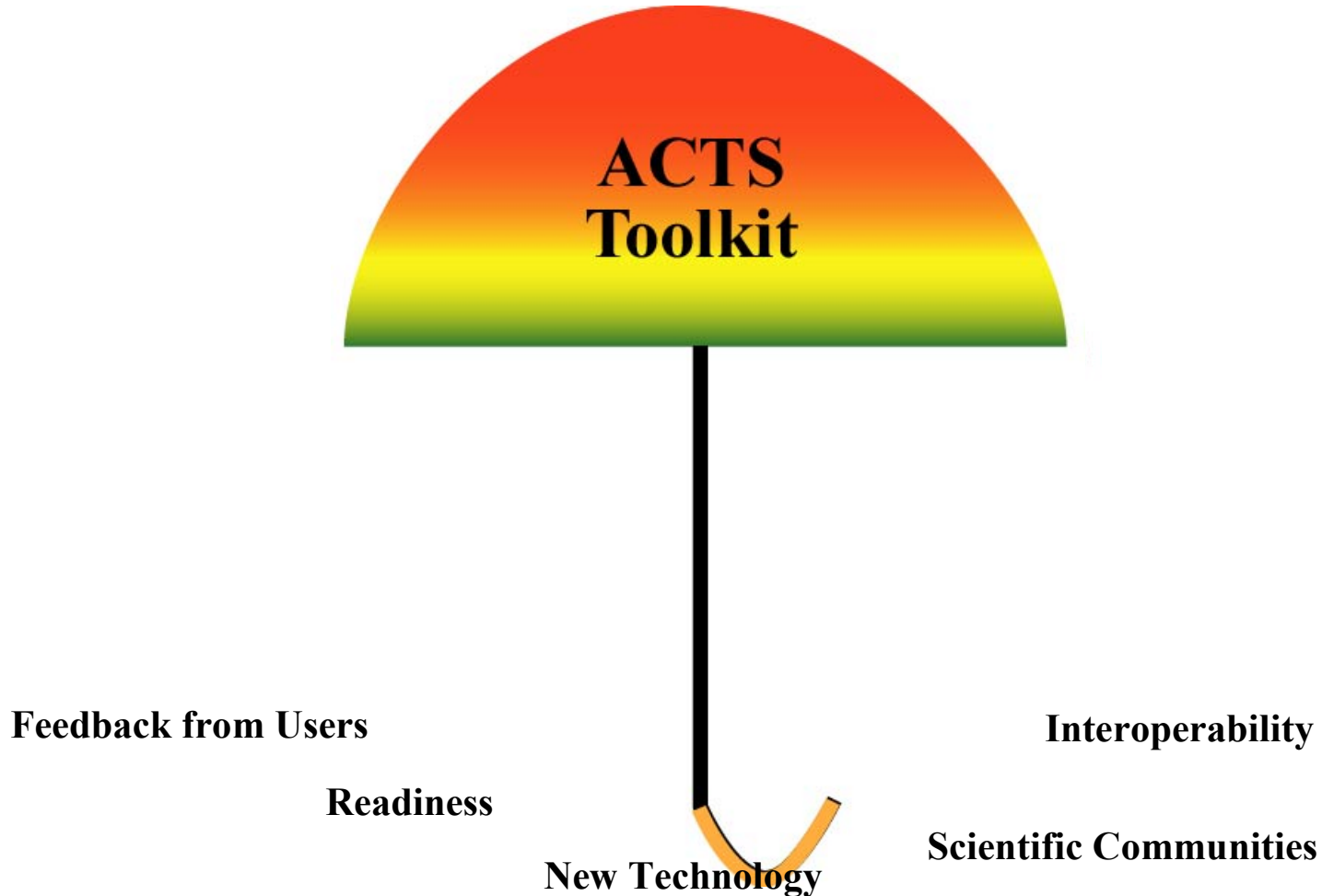
CPU vs. DRAM Performance

- Since 1980's, µProcs performance has increased at a rate of almost 60%/year

Grows
50%/year

- Since 1980's, DRAM (latency) has improved at a rate of almost 9%/year

- Software required to bridge this gap
    - Tuned or optimized to existing hardware capabilities
    - Handle user needs (computational sciences)
    - Portable + Interoperable

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ACTS Toolkit

Feedback from Users

Readiness

New Technology

Interoperability

Scientific Communities

- Visitor program

- Scientific Collaborations

- Tool Development and collaborations

- Reaching out other communities

  - Supercomputing centers

  - Industry (computer and others)

  - Conferences

  - Workshops

- Next round participation

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